Finite Element Model Characterization Of Nano-Composite Thermal And Environmental Barrier Coatings

Thermal and environmental barrier coatings have been applied for protecting Si based ceramic matrix composite components from high temperature environment in advanced gas turbine engines. It has been found that the delamination and lifetime of T/EBC systems generally depend on the initiation and propagation of surface cracks induced by the axial mechanical load in addition to severe thermal loads. In order to prevent T/EBC systems from surface cracking and subsequent delamination due to mechanical and thermal stresses, T/EBC systems reinforced with nano-composite architectures have showed promise to improve mechanical properties and provide a potential crack shielding mechanism such as crack bridging. In this study, a finite element model (FEM) was established to understand the potential beneficial effects of nano-compsoites systems such as SiC nanotube-reinforced oxide T/EBC systems.
Finite Element Model Characterization of Nano-Composite Thermal and Environmental Barrier Coatings

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Introduction

- Environmental barrier coating (EBC) systems are used for protecting Si-based ceramic hot section components.
- Nanotube composites, having extremely high stiffness and strength and functional properties, are currently being considered for EBC to improve the coating performance.
- In particular, SiC nanotubes (SiCNTs) are being incorporated into EBC bond coats to increase their strength and toughness.
Advantages of Nanotube Reinforcements

Nanotubes as compared to other micro scale reinforcements:

- Can achieve much higher volume fraction
- More crack arresters due to more interfaces
- Exhibit more homogenized material response
- Less stress concentration (Gradual stress distribution)

<table>
<thead>
<tr>
<th></th>
<th>Fiber</th>
<th>Wisker</th>
<th>Nanotube</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vf=20%</td>
<td>20 μm</td>
<td>1~5 μm</td>
<td>0.005~0.1 μm</td>
</tr>
<tr>
<td>r</td>
<td>25 μm</td>
<td>1.3~6.5 μm</td>
<td>0.0065~0.130 μm</td>
</tr>
<tr>
<td>Spacing</td>
<td>2~3</td>
<td>8~50</td>
<td>800~4000</td>
</tr>
</tbody>
</table>
Improvement of toughness with SiCNT

HfO$_2$-SiCNT nano-composites, tested at 1450°C ($\Delta T=1000$°C), with Random orientation SiCNT, Wavy, 5 µm long:

- HfO$_2$ + 0% SiCNT:
- HfO$_2$ + 20% SiCNT:
- HfO$_2$ + 40% SiCNT

➢ Higher volume fraction showed improved toughness/strength
Outline

To understand mechanical improvement in toughness/strength

• Multiscale modeling approach for nano-composite property determination:
  ○ HfO₂ + SiCNT nano-composite model system

• FEA to determine micro (nano) scale properties

• Homogenization technique – Micromechanics Analysis Code (MAC/GMC)

• Results and discussions on effect of SiCNT architectures

• Summary
Approach to Determine Global Scale Mechanical Properties

\[ K = \sigma (\pi a)^{1/2}, \text{ where } \sigma = f (E, \Delta T, \ldots) \]

- Increasing stiffness \( E \) will improve toughness \( K \) for a given material system
- Multi-scale modeling approach is used to determine bulk composite stiffness
FEA Simulation (Micro scale properties)

- Assuming perfect bond and equally distributed
- SiCNT: $E_{NT} = 600\text{GPa}$, $\nu = 0.3$
- HfO$_2$ Matrix: $E_m = 100\text{ GPa}$, $\nu = 0.3$
- SiCNT radius: $r = 0.05\ \mu m$ (50 nm)
- SiCNT length: $L = 0.5, 1, 5, 10, 50\ \mu m$
  (r/L=10, 20, 100, 200, 1000)
- Waviness: $\lambda = a/b = 0.0, 0.1, 0.2$
- Orientation: $\theta = 0, 30, 45, 60, 90^\circ$
- Volume fraction: $V_f = 0\sim 60\%$

**FEA model:**

Element Type: Hex20 and Wedge15

# of Nodes: 3000 ~ 90000

# of Elements: 400 ~ 15000
Micro Scale Properties: $V_f$ and Length effect

**FEA simulation**

Straight SiCNT:

Radius: $r = 0.05 \mu\text{m}$
Length: $L = 0.5 \mu\text{m}$

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**Loading direction**

**Transposed direction**
Micro Scale Properties: Effect of Waviness

FEA simulation

$V_f = 20\%$

$\lambda = 0.1$

$\lambda = 0$

$\lambda = 0.2$

$\lambda = 0.1$

$\lambda = 0$

Length of SiCNT, $\mu$m

E/E_M

Loading direction

Transposed direction
Micro Scale Properties: Summary (FEA simulation)

\[ V_f = 20\% \]
\[ \text{SiCNT} \]
\[ L = 5 \mu \text{m} \]

\[ V_f = 40\% \]
\[ \text{SiCNT} \]
\[ L = 5 \mu \text{m} \]
Homogenization (Micro to Macro by MAC/GMC)

- **1st order Taylor series of displacement field**
- **Satisfy continuity of displacements & tractions between subcells**
- **Impose periodicity conditions on displacements and tractions at the unit cell boundaries**

**Triple Periodicity**

- **1st order Taylor series of displacement field**
- **Satisfy continuity of displacements & tractions between subcells**
- **Impose periodicity conditions on displacements and tractions at the unit cell boundaries**

**Double Periodicity**

- Macro-level Constitutive Equations
  \[
  \bar{\sigma} = B^* (\bar{\varepsilon} - \bar{\varepsilon}^T + \bar{\varepsilon}^T)
  \]
  \[
  B^* = \frac{1}{dhl} \sum_{a=1}^{N_a} \sum_{b=1}^{N_b} \sum_{l=1}^{N_l} d_a h_b l_l C^{(a\beta l)} A^{(a\beta)}
  \]
  \[
  \bar{\varepsilon}^l = -\frac{B^{-1}}{dhl} \sum_{a=1}^{N_a} \sum_{b=1}^{N_b} \sum_{l=1}^{N_l} d_a h_b l_l C^{(a\beta l)} (D^{(a\beta l)} \bar{\varepsilon}_S^l - \bar{\varepsilon}^{l(l\beta)})
  \]
  \[
  \bar{\varepsilon}^T = -\frac{B^{-1}}{dhl} \sum_{a=1}^{N_a} \sum_{b=1}^{N_b} \sum_{l=1}^{N_l} d_a h_b l_l C^{(a\beta l)} (D^{(a\beta l)} \bar{\varepsilon}_S^T - \bar{\varepsilon}^{T(l\beta)})
  \]

- Micro-level Field Equations (subcell)
  \[
  \bar{\varepsilon}^{(a\beta l)} = A^{(a\beta l)} \bar{\varepsilon} + D^{(a\beta l)} (\bar{\varepsilon}_S^l + \bar{\varepsilon}_S^T)
  \]
  \[
  \bar{\sigma}^{(a\beta l)} = C^{(a\beta l)} [A^{(a\beta l)} \bar{\varepsilon} + D^{(a\beta l)} (\bar{\varepsilon}_S^l + \bar{\varepsilon}_S^T) - (\bar{\varepsilon}^{l(l\beta)} + \bar{\varepsilon}^{T(l\beta)})]
  \]

Homogenization (Micro to Macro by MAC/GMC)

Double Periodicity

Triple Periodicity

Straight SiCNT:
Radius: \( r = 0.05 \, \mu m \)
Length:
\( L = 0.5, 1.0, 5, 10, 50 \, \mu m \)

MAC/GMC

Longer SiCNT
Shorter SiCNT

\( E/E_M \)

Volume fraction, %

0.8 1.0 1.2 1.4 1.6 1.8 2.0

2.2 2.4 2.6 2.8 3.0

0 10 20 30 40 50 60
Macro Scale Properties for SiCNT Composites

For L = 5 μm:
- $V_f = 40\%$ SiCNT: $\sigma/\sigma_M = 2.02$
- $V_f = 20\%$ SiCNT: $\sigma/\sigma_M = 1.67$

For L = 50 μm:
- $V_f = 40\%$ SiCNT: $\sigma/\sigma_M = 2.07$
- $V_f = 20\%$ SiCNT: $\sigma/\sigma_M = 1.68$
Improvement of toughness with SiCNT

HfO$_2$-SiCNT nano-composites, tested at 1450°C ($\Delta T=1000°C$), with Random orientation SiCNT, Wavy, 5 $\mu$m long:

$$K = \sigma (\pi a)^{1/2}, \text{ where } \sigma = f (E, \Delta T, \ldots)$$

<table>
<thead>
<tr>
<th>Composition</th>
<th>Toughness Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>HfO$_2$ + 0% SiCNT</td>
<td>E = $E_m = 100$ GPa</td>
</tr>
<tr>
<td>HfO$_2$ + 20% SiCNT</td>
<td>E = 1.67~1.68 $E_m$</td>
</tr>
<tr>
<td>HfO$_2$ + 40% SiCNT</td>
<td>E = 2.02~2.07 $E_m$</td>
</tr>
<tr>
<td></td>
<td><strong>Toughness improvement:</strong></td>
</tr>
<tr>
<td></td>
<td>less than +67~68 %</td>
</tr>
<tr>
<td></td>
<td>more than +102~107 %</td>
</tr>
</tbody>
</table>
Summary

- Based on micromechanics modeling, relative improvement in toughness was investigated.

- $V_f$ of 20~40% showed optimum improvement in material properties

- Waviness tends to improve transverse stiffness

- $r/L$ (NT radius to length) ratio > 100 showed no improvement in stiffness

- Totally random orientation with wavy and straight NT provided isotropic material behavior

- Based on preliminary experiments, in order to prevent from surface cracking, 40% $V_f$ of SiCNT (+102% toughness improvement) is needed and 20% $V_f$ (+67% toughness improvement) was not sufficient
Future Work

• Conduct classical fracture test (3pt bend specimen) and indentation test to measure fracture toughness
• Determine SiCNT strength and interfacial bonding strength from Molecular dynamics (MD) simulation

Acknowledgement

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